Outline for Leo – MRes Project 2021/22

# Aim

To improve our model for best ATM design

* To test batch vs column

# Objective

## Coding

* Transfer MATLAB code to Python
  + The MATLAB code in Jay’s thesis and in the Supporting Information of the JECE paper (find the supporting information from the Journal’s webpage) basically takes the column adsorption kinetics equation that we propose in the JECE paper and solves this differential equation through integrating many tiny time steps (using the ODE45 function in MATLAB – Python should have a similar function). The rest of the code basically just runs the simulation many times with slightly different input variables (such as arsenic concentration in the water entering the filter, and different flow rates) and collects the results in a big spreadsheet).
* Extend existing code with adsorption isotherms
  + JECE paper already includes adsorption isotherms
* Plots relevant breakthrough curves
  + Try to simulate the same results as we see in the JECE paper
* Validation and comparison with Jay calculations from paper
* Add new capabilities to optimise the model parameters (such as rate constant k and adsorption capacity Qe) so that we can improve the goodness-of-fit (using R^2 or the Root Mean Square Error) between the model and experimental data.
  + We can find 3 literature papers where they report (1) adsorption isotherms, (2) adsorption kinetics in batch experiments, and (3) breakthrough curves for adsorption columns. We then would take the experimental parameters from (1) and (2), use these to simulate a column experiment, then optimise experimental parameters to improve the goodness-of-fit between the model and the raw data in (3).
* Create a data base for selected mineral-sorbent system

## Scientific

* Create a data base of comparable rates for selected metal – sorbent systems
* To what extent do the experimental parameters from batch experiments (adsorption capacity Qe, rate constant k, and adsorption isotherm parameters) work for the column breakthrough curves? How much do they have to be modified (optimised) to fit the experimental data better?
* Extent approach to photo kinetic reactions and include adsorption isotherms
* Test conclusions from paper

# First steps

1. ~~Read Journal of Journal of Environmental Chemical Engineering~~
2. ~~Read Jay thesis for background on sorbents in water remediation~~
3. Set up a workflow
4. Outline the project proposal
5. ~~Set up GitHub~~
6. Translate MATLAB code to Python and tidy up = make good documentation

1. Reproduce our results from journal (simulation)
2. Find 3 paper sorbent characterisation – adsorption isotherms (see Fig 1 in paper), adsorption kinetics (see Fig 2 in paper and Langmuir paper – talk to Yanan) and column adsorption (see figures
3. Take parameters and run them and look if we can reproduce
4. Then try to develop/test different optimisation techniques to improve parameter (least square, MC)
5. Lit review on modelling batch and columns
6. Identify characterisation papers that have experimental data – test
7. Integrate the MC optimisation – see Yanan – later stage

# Organisation

* Weekly meetings with Dominik (Thursday at 12.30)
* Biweekly meetings with Jay and Kerry
* Get feedback from James re coding
* GitHub to organise our files